

Revisiting the Fermi Golden Rule: Quantum Dynamical Phase Transition as a Paradigm Shift

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Classical and quantum phase transitions involve observables which are non-analytic as functions of a controlled thermodynamical variable. As occurs with the self-consistent Fermi Golden Rule, one condition to obtain the discontinuous behavior is the proper evaluation of a classical or quantum thermodynamic limit. We show that in presence of an environment, the oscillatory dynamics of a quantum two-level system, in analogy with a classical damped oscillator, can undergo a quantum dynamical phase transition to a non-oscillatory phase. This is obtained from a self-consistent solution of the Generalized Landauer Büttiker Equations, a simplified integral form of the Keldysh formalism. We argue that working at each side of the transition implies standing under different paradigms in the Kuhn's sense of the word. In consequence, paradigms incommensurability obtains a sound mathematical justification as a consequence of the non-analyticity of the observables. A strong case is made upon the need to deepen the public's intuition and understanding on the abrupt transition from static to dynamical friction regimes.

key-words: Paradigm Shift, Quantum Dynamical Phase Transition, Dissipative Two-Level Systems, Self-Consistent Fermi Golden Rule, thermodynamic limit

1. Introduction

From metal and glass melting to steam engines, phase transitions have nurtured both technological and scientific progress. Only in the last century has it become clear that phase transitions occur when the relevant free energy is non-analytic on some controlled thermodynamical variables such as the temperature. However, it is not trivial to see how this collective behavior emerges from the fundamental interactions governing microscopic variables. More recently, quantum phase transitions [1], which are much more elusive, have received an increasing interest. This is mainly motivated by the High-Tc superconductors, transport in heavy fermion compounds and organic conductors and condensation of bosonic fluids. The greatest achievement was perhaps the theory of the extended-localized transition of electrons in disordered solids discovered by P. W. Anderson in 1958 [2]. The whole solid state community was taken by surprise by his statement that non-interacting electronic or

vibrational eigenstates in solids would transform from Bloch plane waves into exponentially localized functions whenever the strength of a homogeneous disorder exceeds a critical value. Typically, one should recognize a phase transition as a non-analytic behavior of the ground state energy or other observable as a function of a control parameter g [1]. This sort of phenomena could trivially occur when the control parameter moves the system through a level crossing. However, this involves a total Hamiltonian of the form $H_1 + gH_2$ with H_1 and H_2 mutually commuting. In finite systems this would be an extremely rare situation, but it becomes more likely when one considers an infinite lattice. In this case, the infinite number of degrees of freedom involved could transform an avoided crossing of the finite system into an actual level-crossing.

In this work we want to discuss how a quantum dynamics of a system can undergo a phase transition. We consider a system tunneling coherently between two levels to form a Rabi oscillation. This system is ubiquitous in Nature [3], but has received renewed attention in quantum informa-

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tion field because it constitutes a swapping gate [4,5,6]. The presence of a quantum environment, requires the solution of the dynamics of open systems [7]. We resort to the Keldysh formalism[8] which, with some simplifying assumptions, becomes the Generalized Landauer-Büttiker Equations [9,10] which can be solved analytically. We find that the oscillatory dynamics can freeze when the interaction with a quantum environment exceeds certain critical strength. This behavior has a close analogy with the transition between dynamical regimes (oscillating-overdamped) undergone by a classical oscillator when friction is increased. Since several of the current descriptions of these phenomena do not point out the conceptual assumptions enabling the phase transition, in this article I will sketch out the calculations focusing on the conceptual conundrums: What is the meaning of a ‘thermodynamic limit’ in classical and quantum mechanics? Why does the quantum description of an open system involve a form of thermodynamic limit, and why can this enable a quantum dynamical phase transition?

Finally, I will conclude with a section associating phase transitions to a paradigm shift in science [11]. Similarly to what occurred with the Aristotelian-Newtonian shift, the mechanistic-probabilistic shift manifested in the well known Loschmidt vs. Boltzmann polemics (that switches between reversible and irreversible mechanics) and the related Zermelo/Poincaré vs. Boltzmann argument on the transition between recurrent and dissipative mechanics[12].

2. Effective Hamiltonians

We are particularly interested in the coherent polarization transfer among two magnetic nuclei, which can be reduced to a non-interacting electron [13] so we will resume the basic formulation of the latter problem [14]. The real symmetric Hamiltonian $\hat{H} = \hat{H}^{(0)} + \hat{V}$, describes the dynamics of two states, $|A\rangle = \hat{c}_A^+ |\emptyset\rangle$ and $|B\rangle = \hat{c}_B^+ |\emptyset\rangle$ which are mixed by a tunneling matrix element

$-V_{AB}$. In matrix representation,

$$\begin{aligned} [\mathbf{H}^{(0)} + \mathbf{V}] \vec{u} &= \varepsilon \mathbf{I} \vec{u} \quad \text{with} \\ \mathbf{H}^{(0)} &= \begin{bmatrix} E_A & 0 \\ 0 & E_B \end{bmatrix} \quad \text{and} \quad \mathbf{V} = \begin{bmatrix} 0 & -V_{AB} \\ -V_{BA} & 0 \end{bmatrix}. \end{aligned} \quad (1)$$

Eliminating one of the amplitudes, e.g. u_B , gives

$$\underbrace{[E_A + V_{AB} \frac{1}{\varepsilon - E_B} V_{BA}]}_{\Sigma_A} u_A = \varepsilon u_A. \quad (2)$$

Obviously the bracket is an ‘effective’ Hamiltonian $H_A^{\text{eff.}} = \bar{E}_A(\varepsilon)$ which includes the ‘energy shift’ $\Sigma_A(\varepsilon)$ due to the eliminated orbital

$$\bar{E}_A(\varepsilon) = E_A + \Sigma_A(\varepsilon), \quad (3)$$

$$\Sigma_A(\varepsilon) = V_{AB} \frac{1}{(\varepsilon - E_B)} V_{BA}. \quad (4)$$

Indeed, under an apparent simplicity, the equation becomes non-linear and it’s solution provides the two exact eigenvalues of the system

$$\varepsilon_A = \frac{1}{2}[(E_A + E_B) - \hbar\omega_{AB}], \quad (5)$$

$$\varepsilon_B = \frac{1}{2}[(E_A + E_B) + \hbar\omega_{AB}] \quad (6)$$

$$\hbar\omega_{AB} = \sqrt{(E_B - E_A)^2 + 4|V_{AB}|^2} \quad (7)$$

This procedure can also be expressed in terms of Green’s functions. Given a positive η , one defines the retarded and advanced resolvent matrices,

$$\mathbf{G}^R(\varepsilon + i\eta) = [\mathbf{G}^A(\varepsilon - i\eta)]^\dagger \quad (8)$$

$$= [(\varepsilon + i\eta) \mathbf{I} - \mathbf{H}]^{-1} \quad (9)$$

$$= \underbrace{\frac{1}{(\varepsilon - E_A)(\varepsilon + i\eta - E_B) - V_{AB}V_{BA}}}_{(\varepsilon + i\eta - \varepsilon_A)(\varepsilon + i\eta - \varepsilon_B)}$$

$$\times \begin{bmatrix} \varepsilon + i\eta - E_B & -V_{AB} \\ -V_{BA} & \varepsilon - E_A \end{bmatrix}. \quad (10)$$

The retarded (advanced) Green’s functions are matrix elements which, for real ε , have divergences at the eigen-energies as $\eta \rightarrow 0^+$ being analytic in the upper (lower) half plane. These divergencies weigh the probability of the unperturbed

state on the eigenstates $|\bar{A}\rangle$ and $|\bar{B}\rangle$. Hence, the local density of states (LDoS) at site $n = A, B$ results:

$$\begin{aligned} N_n(\varepsilon) &= -\frac{1}{\pi} \lim_{\eta \rightarrow 0^+} \text{Im} \langle n | \hat{G}^{oR}(\varepsilon + i\eta) | n \rangle \quad (11) \\ &= -\frac{1}{2\pi} [G_{n,n}^{oR}(\varepsilon) + G_{n,n}^{oA}(\varepsilon)] \\ &= |\langle n | \bar{A} \rangle|^2 \delta(\varepsilon - \varepsilon_A) + |\langle n | \bar{B} \rangle|^2 \delta(\varepsilon - \varepsilon_B). \end{aligned}$$

The diagonal matrix elements can be rewritten as

$$G_{A,A}^R(\varepsilon) = \frac{1}{\varepsilon - \bar{E}_A(\varepsilon)}, \quad (12)$$

Identifying the unperturbed Green's functions $G_{n,n}^{oR}(\varepsilon) = [\varepsilon - E_n]^{-1}$ and expanding one gets,

$$\begin{aligned} G_{A,A}^R(\varepsilon) &= \frac{1}{[G_{A,A}^{oR}(\varepsilon)]^{-1} - \Sigma_A(\varepsilon)} \\ &= G_{A,A}^{oR}(\varepsilon) + G_{A,A}^{oR}(\varepsilon) \Sigma_A(\varepsilon) G_{A,A}^{oR}(\varepsilon) \\ &\quad + G_{A,A}^{oR}(\varepsilon) \Sigma_A(\varepsilon) G_{A,A}^{oR}(\varepsilon) \quad (13) \\ &\quad \times \Sigma_A(\varepsilon) G_{A,A}^{oR}(\varepsilon) + \dots \end{aligned}$$

This shows that the exact solution is the sum of an infinite geometric series. This is represented as Feynman diagrams in Fig. 1. There is yet another form of writing this, a Dyson equation,

$$G_{A,A}^R(\varepsilon) = G_{A,A}^{oR}(\varepsilon) + G_{A,A}^R(\varepsilon) \Sigma_A(\varepsilon) G_{A,A}^{oR}(\varepsilon). \quad (14)$$

It is useful to note that all the above results, and most of what follows, are also valid if $|A\rangle$ and $|B\rangle$ denote whole subspaces. In that case, all the presented equations and diagrams hold but with matrix elements transformed themselves into matrices[15,16]. We might choose not to deal explicitly with an undesired subspace, for example the whole subspace $|B\rangle$, and still get an effective Hamiltonian restricted to the subspace $|A\rangle$ and also the exact Green's function.

Usually, given an initial state, the dynamics is evaluated from eigen-energies and eigenstates. Alternatively, it can be expressed in terms of Green's functions. For example, the probability

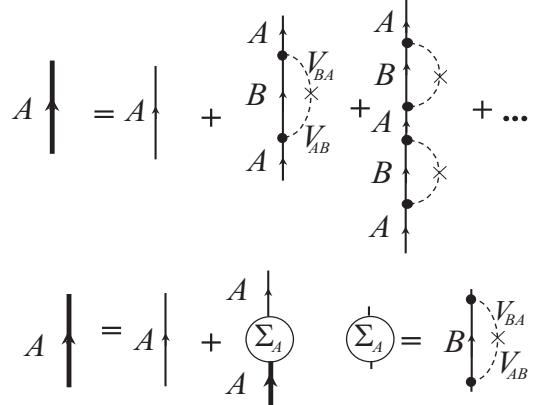


Figure 1. In the upper panel, the exact Green's function (thick line) is represented as an infinite series of unperturbed Green's functions (thin lines). Coupling matrix elements are dashed lines. The bottom panel shows the self-consistent Dyson equation and the self-energy.

that a particle which was in the state $|A\rangle$ at $t = 0$ is found at state $|B\rangle$ at a later time t results:

$$P_{B,A}(t) = \left| \langle B | \exp[-i\hat{H} t] | A \rangle \right|^2 \theta[t] \quad (15)$$

$$= \left| \lim_{\eta \rightarrow 0^+} \int \frac{d\varepsilon}{2\pi\hbar} G_{B,A}^R(\varepsilon + i\eta) \exp[-i\varepsilon t] \right|^2 \quad (16)$$

$$= \int \frac{d\omega}{2\pi} \exp[-i\omega t] P_{B,A}(\omega) \quad (17)$$

$$= \int d\varepsilon P_{B,A}(\varepsilon, t), \quad (18)$$

with

$$P_{B,A}(\omega) = \int d\varepsilon \overbrace{G_{B,A}^R(\varepsilon + \frac{1}{2}\hbar\omega) G_{A,B}^A(\varepsilon - \frac{1}{2}\hbar\omega)}^{P_{B,A}(\varepsilon, \omega)}. \quad (19)$$

The appearance of the function $\theta[t]$ in Eq. 15 is consequence of the election of the sign of the imaginary part in the retarded Green's function.

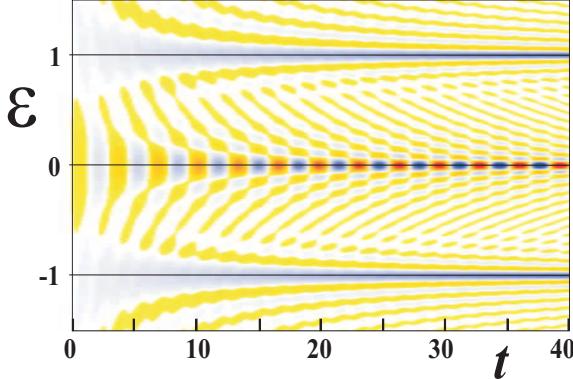


Figure 2. (Color online) Energy-time distribution function for a two-level system (in units of V and \hbar/V respectively) The dark (yellow-red online) and clear (blue online) regions differ in sign. The formed stripes manifest the progressive decrease in the small structure's scale as function of time.

The remaining two lines constitute alternatives for writing the product of the independent integrals. The function $P_{B,A}(\varepsilon, t)$ (as well as its transform $P_{B,A}(\varepsilon, \omega)$) is not an actual probability but a form of energy-time distribution function from which a real probability can be obtained as a marginal distribution, i.e. by integration of one of the variables. In more general problems, this energy-time distribution enabled [9,10] to consider time dependent statistical distribution functions. For the particular case of equal energies $E_A = E_B = 0$ and $V_{AB} = V$ with the superposition $|A\rangle = \frac{1}{\sqrt{2}}(|\bar{A}\rangle + |\bar{B}\rangle)$ as initial state:

$$P_{A,A}(\varepsilon, t) = \frac{V^2 + \varepsilon(V - 2\varepsilon)}{2\varepsilon(V^2 - \varepsilon^2)} \sin[2(\varepsilon + V)t] \theta(t) \quad (20)$$

$$+ \frac{V^2 - \varepsilon(V + 2\varepsilon)}{2\varepsilon(V^2 - \varepsilon^2)} \sin[2(\varepsilon - V)t] \theta(t)$$

This distribution oscillates as a function of each participant energy at a rate which is determined by its distance to the eigenvalue (see Fig. 2). From it, the Rabi oscillation is obtained as:

$$P_{A,A}(t) = \int d\varepsilon P_{A,A}(\varepsilon, t) = \cos^2(\frac{1}{2}\omega_{AB}t). \quad (21)$$

Notice that while the result of the integral remains a simple oscillation, for long times the integrand becomes an increasingly oscillatory function on the energy variable. In a numerical integration, regions with too small structures would contribute as pseudo-random amount to the integral making it numerically unstable. It would be tempting to do an analogy with similar structures in the standard momentum-position Wigner function suggested by Zurek [17,18], and interpret this phenomenon as a manifestation of the instability of this quantum superposition towards decoherence. In fact, ideal Rabi oscillations contrast with experimental observations, such as Fig. 4-a of Ref. [19], where the environment is actually attenuating the oscillation while the probability is conserved. Thus, our simple quantum mechanical model should be extended to include some form of environmental interaction.

3. The spectrum of a finite linear chain and continued fractions.

We will represent the environment with our favorite model, the linear chain. It not only represents a chain of spins interacting through a XY interaction[20] but it is a reasonable model for polymers, quasi-one dimensional crystals and metal wires. Even a crystal structure can be reduced to a set of uncoupled linear chains. We start by adding a third state to our two state system,

$$\mathbf{H} = \begin{bmatrix} E_1 & -V_{12} & 0 \\ -V_{21} & E_2 & -V_{23} \\ 0 & -V_{32} & E_3 \end{bmatrix}. \quad (22)$$

We start with $V_{12} = 0$. Through the identification of the indices $2 \rightarrow A$, and $3 \rightarrow B$, we use Eq.3 eliminate state B (i.e.3) so that $G_{A,A}^R(\varepsilon) \rightarrow \bar{G}_{2,2}^{oR}(\varepsilon)$. Now we turn-on $V_{1,2}$ and identify $1 \rightarrow A$ and $2 \rightarrow B$, and we repeat the elimination of B to get:

$$G_{1,1}^R(\varepsilon) = \frac{1}{[G_{1,1}^{oR}(\varepsilon)]^{-1} - V_{12}\bar{G}_{2,2}^{oR}(\varepsilon)V_{21}} \quad (23)$$

We replace it and obtain a nested fraction:

$$G_{1,1}^R(\varepsilon) = \frac{1}{\varepsilon - E_1 - V_{12} \underbrace{\frac{1}{\varepsilon - E_2 - V_{23} \underbrace{\frac{1}{\varepsilon - E_3} V_{32}}}_{\Sigma_2}}_{\Sigma_1}} \quad (24)$$

In the present context, the self-energy accounts for presence of states at the right.

Hamiltonian of Eq. (22) presents an interesting phenomenon. If $V_{23} \ll V_{12} = V_{AB}$ the system AB is well defined and site 3 can be seen as an “environment” weakly perturbing the system through $V_{SE} = V_{23}$. If we allow the parameters to switch to the opposite regime $V_{SE} = V_{23} \gg V_{12} = V_{AB}$, state B becomes “captured” by the environment and the state A becomes almost isolated. This can be seen as a form of the Quantum Zeno Effect [21] caused by the internal degrees of freedom [22,23].

Since the procedure performed above was in fact a step of a renormalization group algorithm[24,15], we can iterate it to get the general continued-fraction that describes a chain with N orbitals:

$$\Sigma_n(\varepsilon) = V_{n,n+1} \frac{1}{\varepsilon - E_n - \Sigma_{n+1}(\varepsilon)} V_{n+1,n}. \quad (25)$$

together with the termination condition.

$$\Sigma_N(\varepsilon) \equiv 0. \quad (26)$$

Hence, the Green’s function, as the self-energy, is the ratio between two polynomials. This yields the N eigen-energies and eigenvalue weights of the finite system. As predicted by Poincaré this produces many recurrences. A particularly interesting dynamical recurrence is what we called [25] the *mesoscopic echo* which appears at the Heisenberg’s time $T_{ME} = \hbar/\bar{\Delta}$ where $\bar{\Delta}$ is the mean level spacing. Signatures of this phenomenon were experimentally observed in Córdoba [20] and confirmed in Zurich by the group of Richard R. Ernst as can be seen in Fig. 3-B of Ref. [26].

4. The semi-infinite ordered chain

When the chain of lattice spacing a is ordered ($E_n \equiv 0$, $V_{n,n+1} \equiv V$) and infinite there is no termination condition as Eq. 26. Instead, all sites “see” the same environment at their right. Hence, the equation that is now equivalent to the Bloch theorem is

$$\Sigma_n(\varepsilon) \equiv \Sigma_{n+1}(\varepsilon) = \Sigma(\varepsilon), \quad (27)$$

from which:

$$\Sigma(\varepsilon) = \frac{V^2}{\varepsilon - \Sigma(\varepsilon)}. \quad (28)$$

The surprise is that in the region where *there are* real eigenvalues, the solution is complex

$$\Sigma(\varepsilon) = \Delta(\varepsilon) - i\Gamma(\varepsilon), \quad (29)$$

the energy shift is a piece-like function:

$$\Delta(\varepsilon) = \begin{cases} \frac{\varepsilon}{2} - \sqrt{\left(\frac{\varepsilon}{2}\right)^2 - V^2} & \text{for } \varepsilon > 2|V|, \\ \frac{\varepsilon}{2} & \text{for } |\varepsilon| \leq +2|V|, \\ \frac{\varepsilon}{2} + \sqrt{\left(\frac{\varepsilon}{2}\right)^2 - V^2} & \text{for } \varepsilon < -2|V|. \end{cases} \quad (30)$$

while the group velocity, $\Gamma = \hbar v_\varepsilon/a$, results

$$\Gamma(\varepsilon) = \begin{cases} 0 & \text{for } \varepsilon > 2|V|, \\ \sqrt{V^2 - \left(\frac{\varepsilon}{2}\right)^2} & \text{for } |\varepsilon| \leq +2|V|, \\ 0 & \text{for } \varepsilon < -2|V|. \end{cases} \quad (31)$$

The sign of the square root is consistent with the analytical properties described above, while the real part goes to zero as $\lim_{\varepsilon \rightarrow \pm\infty} \Delta(\varepsilon) = 0$ which means that the spectrum of the linear chain remains bounded after the interaction has been turned-on. The consistency of these solutions can be checked through the convergence of the self-energies in chains of increasing lengths. This expresses the *Quantum Thermodynamic Limit*:

$$-\Gamma(\varepsilon) = \lim_{\eta \rightarrow 0^+} \lim_{N \rightarrow \infty} \text{Im} \Sigma_1(\varepsilon + i\eta) \quad (32)$$

$$\neq \lim_{N \rightarrow \infty} \lim_{\eta \rightarrow 0^+} \text{Im} \Sigma_1(\varepsilon + i\eta) \underset{\text{a.e.}\varepsilon}{\equiv} 0 \quad (33)$$

a.e. ε means for almost every ε , i.e. except for a set whose probability measure is zero. The non-triviality of this limit is manifested in the fact that it is non-uniform.

5. The Fermi Golden Rule as a Quantum Thermodynamic Limit

In the above discussion we obtained an effective energy with an imaginary component. It actually means that perturbation theory does not converge. The unperturbed eigenstate is so far from the new eigenstates that their scalar product vanishes. In the dynamics, this should manifest as a progressive decay where the Poincaré recurrences no longer appear. This means that the probability escapes towards the semi-infinite chain. For the homogeneous linear chain this involves a power law decay according to the law $P_{1,1}(t) \simeq (Vt)^{-1}$. A particularly interesting case occurs when at the end (surface) of this semi-infinite chain we add an orbital (or atom) with energy E_0 and interaction $V_0 \ll V$. This adatom model, is a particular case of the Friedrichs model. One knows that this situation leads to a typical exponential decay described by the Fermi Golden Rule (FGR). However, a deeper analysis shows that the exact rate of decay differs from that in the FGR. The new rate, Γ_0/\hbar , arises from a Self Consistent Fermi Golden Rule [27]. It is the imaginary part at the exact pole $\varepsilon_r - i\Gamma_o$ of the Green's function:

$$\varepsilon_r - i\Gamma_0 = E_0 + \frac{V_0^2}{V^2} \Sigma(\varepsilon_r - i\Gamma_o) \quad (34)$$

which can be obtained analytically or by iteration.

One should not forget that a quantum decay starts always quadratically, in this case with a time scale \hbar/V_0 . It only starts looking exponential after a time t_S . This is a short time scale,

$$t_S = \hbar\pi \bar{N}_1(\varepsilon_r), \quad (35)$$

when the escape from the surface site towards the rest of the chain prevents the return and hence stops giving an appreciable contribution to the survival. Here, $\bar{N}_1(\varepsilon_r)$ is the LDoS at the surface site in absence of the adatom. At times longer

than,

$$t_R = \alpha \frac{\Gamma_0}{\hbar} \ln \left[\beta \frac{B}{\Gamma_0} \right], \quad (36)$$

the return amplitude, determined by the high order processes that has already escaped but remains in the neighborhood, starts being comparable to the pure survival amplitude. From then on, decay becomes a power law $[\Gamma(\varepsilon_r)t]^{-3/2}$. Here, $B = 4V$ is the bandwidth and $\alpha, \beta \gtrsim 1$ are constants that depend on the van Hove singularities of $\bar{N}_1(\varepsilon_r)$ and other details of the model. At t_R a striking destructive interference between the pure survival amplitude and the return amplitude may occur. In quantum systems, this “survival collapse” [27] has yet to be observed.

In summary, the validity of the FGR is restricted by memory effects to times between t_R and t_S . The standard FGR holds in the wide band limit $\Gamma_0/B \rightarrow 0$ which also implies that $V_0 \bar{N}_1(\varepsilon_r) \rightarrow 0$. It is only in this condition, valid in a quite broad variety of situations, that one can forget the quantum memory effects of a finite bandwidth and replace both $\Delta(\varepsilon) - i\Gamma(\varepsilon)$ by $\Delta - i\Gamma$ independent of ε . The environment behaves as a Markovian process and we refer to them as the “broad band approximation” or “fast fluctuations approximation”. One should be careful, however, interpreting this as an “irreversible” behavior [28]. Actual irreversibility is consequence of an instability that manifests when one attempts to revert the dynamics through a “Loschmidt daemon”, $\hat{H} \rightarrow -\hat{H}$ [29]. One should note that an imaginary part by itself does not ensure irreversibility as long as one can change the sign of the whole Hamiltonian. The instability of this procedure can be tested and quantified through the Loschmidt echo (or fidelity) in spin dynamics [30,31], confined atoms [32] and microwaves in cavities [33]. See also Ref. [34] for a completely different approach to achieve time-reversal.

The physical meaning of the imaginary part we introduced at the beginning is now evident: it represents the weak interaction with an environment. In such situation, Δ does not contribute much to the dependence on ε and one includes it by shifting the energies. This approximation

would give a steady decay of the Rabi oscillation as is indeed typical of many experimental setups. See for example the Fig. 4-a in Ref [19]. However, one might wonder how to return the probability lost in this decay. In fact in presence of two identical linear chains connected to states A and B , one would find probability [35],

$$\begin{aligned} \bar{P}_{A,A}(t) &= P_{A,A}(t) \exp[-2\Gamma t/\hbar] \\ &= \cos^2(2\omega_{AB}t) \exp[-t/\tau], \text{ with } \tau = \hbar/2\Gamma. \end{aligned} \quad (37)$$

Clearly, this describes the evolution of polarization tunneling between two nuclei shown in Fig. 4.b of Ref. [19]. In this case, the probability (polarization) is not conserved but it decays according to the FGR. While this could be correct in some physical situations, the description of a situation closer to Fig. 4.a, where probability is conserved, remained a challenge.

6. The Generalized Landauer-Büttiker Equation

The imaginary energy has been a puzzle for everyone using Green's functions and regularizing its poles. Sometimes, as in the electron-phonon processes, an explicit form for this imaginary energy is evaluated through the FGR. Even the transport equations, as the Kubo formula, rely on some natural broadening which enables the computation but produces local non-conservation of currents. The answer was given by D'Amato and Pastawski [36] who, extending an idea of Büttiker[37], realized that the escape to an environment is equivalent to saying that, at each time, a fraction of the system occupation escapes to the chain which could act as a voltmeter. As an actual voltmeter, however it should not extract net particles from the system, so it returns a particle for each one collected. This can be expressed [9] in terms of the Landauer description of transport which now accounts for time dependences and decoherent process in the form of a Generalized Landauer-Büttiker Equation (GLBE). Hence, for every process of "escape" from the coherent beam due to the interaction with the environment, a fresh incoherent particle must be reinjected into the system as expressed in Eq. (3.7) of Ref. [9].

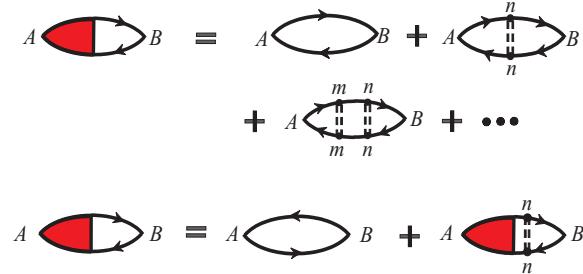


Figure 3. Diagrams for the density propagator from A to B as dictated by Generalized Landauer-Büttiker Equation. Horizontal lines are single particle Green's functions dressed by the environment. Shadowed vertices are the self-consistent density propagators. The vertical double dashed lines represent the reinjection processes. The last collision occurs at site n .

This physical picture, finds its formal justification when the system-environment interactions are local and the environment spectrum is so broad that it becomes instantaneous and energy independent. In this case, the Keldysh quantum field theory formalism, expressed in its integral form [38], reduces to the GLBE [10,14] represented in Fig. 3.

We consider a degenerate two-level system where, besides tunneling, each state suffers the action of a complex self-energy, such as that of the linear chain described in the previous section. This results in an homogeneous interaction with the environment. The natural parameter regulating the effectiveness of the system-environment is $g = \omega_{AB}\Gamma/\hbar$. For this two-level system the GLBE becomes:

$$\begin{aligned} \tilde{P}_{A,A}(t) &= \bar{P}_{A,A}(t) \\ &+ \sum_{n=A,B} \int_0^{t_i} \bar{P}_{A,n}(t - t_i) \frac{dt_i}{\tau} \tilde{P}_{n,A}(t_i), \end{aligned} \quad (38)$$

and equivalent equations for the components BA , AB and BB . This is a Volterra's type equation. This is a Dyson equation (much as Eq. 14) for

a density, i.e. a two-particle Green's function, and is also known as a Bethe-Salpeter equation. The first term describes the probability of coherent propagation from the initial to the final state which decays due to interactions with the environment. The kernel of this equation is precisely $\tilde{P}_{A,n}(t - t_i)$, the two-particle propagator. Since dt_i/τ is the probability of having the last interaction with the environment at the time interval dt_i around t_i . The solution of the homogeneous GLBE can be obtained by Fourier transformation [39] $\tilde{P}_{B,A}(\omega)$ and decays toward the equilibrium $\tilde{P}_{B,A}(t) \rightarrow \frac{1}{2}$. One notable thing is that the first term in the right has poles in the complex ω -plane that correspond to the difference of energies and do not present any form of non-analyticity. The self-consistent solution $\tilde{P}_{B,A}(\omega)$ has more information. In fact, the poles of $\delta\tilde{P}_{B,A}(\omega) = \tilde{P}_{B,A}(\omega) - \frac{1}{2}\delta(\omega)$ are precisely at

$$\omega^\pm - i\Gamma = \pm\sqrt{[\omega_{AB}]^2 - \Gamma^2} - i\Gamma \quad (39)$$

The trajectories in the complex plane are shown in Fig. 4-b. The important feature is that the real part of the poles (Fig. 5-a) collapses at 0 for a critical value $g_c = 1$ and from this point they split in two terms of null real part. One of them decreases with environment interaction whereas the other decreases. It is the later that controls the long time behavior.

$$\delta\tilde{P}_{A,A}(t) = \tilde{P}_{A,A}(t) - \frac{1}{2} = a_0 \cos [(\omega + i\Gamma)t + \phi]. \quad (40)$$

Here $P_{A,A}^{\text{eq.}} \equiv \frac{1}{2}$ is the equilibrium occupation while $a_0^2 = [4\omega^2\tau^2 + 1] / (16\omega^2\tau^2)$ and $\phi = \arctan[1/2\omega\tau]$ warrant the initial quadratic decay.

The described behavior has been experimentally observed in heterogeneous polarization transfer, see Fig. 7 of Ref. [30], but overlooked since the early theory for this experiment [40] did not contain the transition. Recent experimental studies [6] show the divergence of the period $2\pi/\omega$ at a critical ratio $\hbar\omega_{AB}/\Gamma = 1$. Conceptually, the transition is from an isolated system that is weakly perturbed to a state in which the

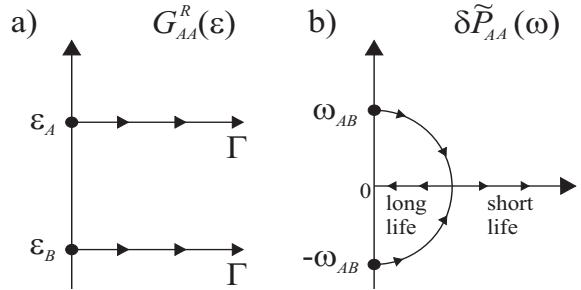


Figure 4. a) Paths of poles of a single particle Green's function, e.g. $G_{AA}^R(\epsilon)$, when an homogeneous decay Γ is increased. They move parallel to the imaginary axis. b) Paths of poles of the observable $\delta\tilde{P}_{B,A}(\omega)$ (a two-particle self-consistent Green's function) when Γ increases. The symmetric frequencies collapse at the center where a branching occurs. One mode becomes long life while the other has a short life time.

effect of the environment is no longer perturbative. The system may be no longer well defined as discussed with reference to Eq. 22. This would be a dynamical Quantum Zeno Effect [22,23]. While the limiting cases were somehow expected, it was by no means obvious that this change could be critical. The non-analyticity was enabled by the infinite degrees of freedom of the environment in the proper quantum thermodynamic limit and the self-consistent nature of Eq. 38.

The excess density $\delta\tilde{P}_{A,A}(t)$ behaves exactly as the amplitude $x(t)$ of a damped classical oscillator which undergoes a transition to an over-damped regime. Indeed, considering a damped harmonic oscillator of mass m and natural frequency ω_o , the relaxation rate as a function of the friction coefficient, Γ , follows precisely the trace of Fig 5-b: The rate increases with friction until a critical value when it starts to decrease inversely proportional to the friction coefficient Γ . This is, of course, a non-analytic critical behavior. Where does it come from? From the imaginary self-energy correction that shifts the nat-

ural frequency ω_0 in the oscillator's dynamical susceptibility $\chi(\omega) = -m^{-1} / [\omega^2 - (\omega_0^2 - i\omega\Gamma)]$. The damped Newton's equation is not a fundamental law but it is written on phenomenological grounds. However, the inclusion of Γ can be justified, within statistical mechanics, by including the action of a Brownian bath [41]. Recently, we obtained a simpler demonstration [42] using as environment a chain of oscillators whose N degrees of freedom are considered by taking the thermodynamic limit of $N \rightarrow \infty$ precisely in the same way as described above in the context of the FGR. It is interesting to note that while $2\omega_0/\Gamma \gg 1$ corresponds to the standard oscillation. In a similar way, in the quantum case $2\omega_0/\Gamma \gg 1$, the system is well defined and the environment is a small perturbation. In contrast in the regime controlled by friction, $2\omega_0/\Gamma \ll 1$, the inertia term can be completely neglected.

It is clear that most of the qualitative features of the spectral properties described above are valid for other linear systems (provided that there is a thermodynamic limit) and hence are ubiquitous in Nature. In magnetic resonance, a phenomenon known as exchange narrowing, has long been described [43] and clearly observed [44]. However, its explanation requires either Brownian fluctuations or the use of Markov chains with imaginary probabilities...! [45].

7. Phase Transitions as Paradigm Shifts

In the previous sections we have touched upon issues such as complex energies, imaginary probabilities, irreversibility, recurrences, decoherence, non-analytic observables, etc., all of them generating strong polemics. In consequence, some epistemological comments are pertinent.

One of the central statements of ancient Physics was Aristotle's dictum that everything that moves is moved by something else. More precisely, Aristotle says that the velocity of a moving object is directly proportional to the force and inversely proportional to the resistance, i.e. $\dot{x} = F/\Gamma$. In the absence of a proximate force, the body would come to rest immediately. Obviously, a difficulty found in the Aristotelian view is the justification of why a projectile keeps moving

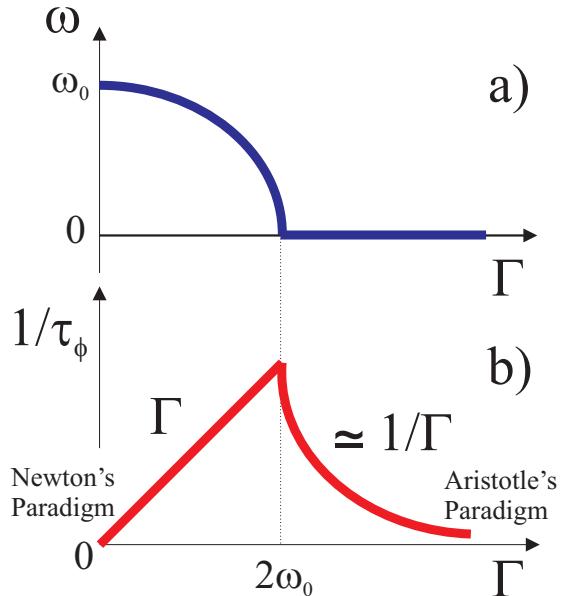


Figure 5. a) The frequency of a two-level system (Fig. 4b) collapses at zero for a critical Γ . b) the decoherence rate as function of Γ . This also represents a relaxation rate in a damped harmonic oscillator as function of friction strength. The bottom left point is ideal frictionless Hamiltonian mechanics or Newton's paradigm. The right side is the realm of Aristotle's paradigm where inertia becomes negligible.

through the air. The logic of the explanation is not as clean as the central statement: a projectile would owe its continuing motion to the force of eddies or vibrations in the surrounding medium, a phenomenon known as antiperistasis. This was formalized later on by the scholastics [47] who proposed that motion was maintained by some property of the body, the *impetus*, which once set in motion, would impart the force keeping the movement. Buridan's *impetus* has the same consequence, but very different justification, than the modern concept of momentum [46].

Physics seemed a quite solid construction until the experiments and intuition of Galileo and

analytical skills of Newton started to build much of our current knowledge. In this new formulation, the *inertia* is no longer a correction but the *fundamental principle*. Friction appears now as a subsidiary and phenomenological effect needed to fit the natural phenomena to the ideal scheme. Indeed its justification remained for a long time alien to Hamiltonian mechanics. One had to wait for the appearance of Boltzmann's statistical mechanics and the work of Smoluchowski and Einstein to have a place in the theory building (for a simple Hamiltonian model justifying friction see Ref. [42]). In any case, Aristotelian and Newtonian views, were so completely irreconcilable that Thomas Kuhn [48] concluded that they were indeed different views of Nature. He coined the term *paradigm shift* to describe a change in the basic assumptions within the ruling theory of science. According to Kuhn, science progress relies not only on a linear accumulation of new knowledge as sustained by Karl Popper but, more fundamentally, on periodic revolutions in which the nature of scientific inquiry within a particular field is abruptly transformed [11]. Rival paradigms are said to be *incommensurable* because it is not possible to understand one paradigm through the conceptual framework and terminology of another rival paradigm.

What seems disturbing to some scientists, is the possibility that no ultimate truth underlies this confrontation between paradigms [49]. Is it possible to synthesize these extreme behaviors into a single framework? Our answer is yes, because incommensurability involves comparing states at different sides of a phase transition. Indeed, Aristotle's paradigm is placed at the extreme right side of Fig. 5-b where the inertia's contribution to an equation of motion is completely neglected. The impetus corrections allows one to move somehow to the left. The contrasting Newton's paradigm, $\ddot{x} = F/m$, is placed at the extreme left, in the origin of Fig. 5-b. From that ideal point one could conceive adding friction as a correction. Consider a mass placed in a bowl where friction can be varied. Would anyone experimenting in one of those extremes conceive, without completing the experiment of the other regime, what the response at the other edge would

be? The answer is a clear no, as the non-analytic function does not allow a natural extrapolation. Indeed, it was not until Gauss popularized the concept and interpretation of Euler's complex numbers that both regimes fitted into a single description. Even with that tool, numerous discussions with students and colleagues convinced me that intuition fails lamentably at the non-analytic point. The same occurs when one discusses problems which involve the non-homogeneity of the limits, which indeed is at the root of the microscopic description of friction. Many other controversies in Physics have a resolution within this framework: we have already advocated that the Loschmidt vs. Boltzmann controversy is a consequence of the non-uniformity of the limits for an imperfect time reversal experiment [31]. Each argument results valid in a different approach to the limiting case (see Fig. 6 in Ref. [18]). The Zermelo/Poincaré-Boltzmann controversy is another consequence of different forms of taking the thermodynamic limit.

More recently, in the quantum framework, the localized-extended transition owes its origin to the fact that strong disorder induces a non-uniformity of the limits respect to ensemble average,

$$\bar{\Gamma}(\varepsilon) = \lim_{\eta \rightarrow 0^+} \left\langle \lim_{N \rightarrow \infty} \text{Im } \Sigma(\varepsilon + i\eta) \right\rangle_{\text{ens. ave.}} \quad (41)$$

$$\neq \left\langle \lim_{\eta \rightarrow 0^+} \lim_{N \rightarrow \infty} \text{Im } \Sigma(\varepsilon + i\eta) \right\rangle_{\text{ens. ave. a.e.}\varepsilon} \equiv 0. \quad (42)$$

This inequality and the last equality were proved and tested numerically in Ref. [50]. They show that in the localized regime the spectrum is pure-point. Not recognizing it led to contradictory results for about two decades [51,52]. Also the coarse grain average has subtle properties of non-uniformity respect to the thermodynamic limit which need further exploration [53].

There are other smaller paradigm shifts in condensed matter physics, which resulted somehow less conflictive, produced by the need to explain quantum phase transitions. We can mention superconductivity (from current carried by single electrons to Cooper's pairs), localization and

mesoscopic transport (which shifted from Kubo's view where dissipation occurs inside the sample to that of Landauer, where it occurs at the external reservoirs) and the Integer Quantum Hall (where the standard vision of bulk current yields to Büttiker's edge current).

Finally, I feel the obligation to mention another phase transition which should not be much different from that discussed above: the transition from static friction to dynamical friction. In that case, ordinates in Fig. 5-b describe the friction force as a function of the applied force. The abrupt fall of the last at a critical force describes the transition to the almost constant value of the dynamical friction. In fact, the non-analytic jump from static friction to dynamical friction is so unexpected and counter-intuitive that no other phase transition seems to have a bigger deathly tall in "accidents" on the road, at work or even at home. It seems to me that it is a most urgent challenge to devise an educational strategy capable to develop, in the general public and physicists alike, an intuition on this phenomenon. On the physical side, friction has only recently been reintroduced as a fundamental problem [54]. Its formulation relies on models having a close connection to issues discussed above [55]. This is still another phase transition that opens new questions not only for basic physics but, even more importantly, also to social and cognitive sciences.

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